



GPU Programming. When, Why and How?

2024

ENCCS Training



Non-portable kernel-based models. Fundamentals

CUDA and HIP



- CUDA and HIP are solely focused on GPUs.
- CUDA and ROCM toolkits provide all the necessary tools and advance features to write highly optimized applications for running on GPUs:
 - optimized libraries
 - low level APIs
 - compiler toolchains that optimize code execution on NVIDIA GPUs (in the case of CUDA) and both NVIDIA and AMD GPUs (in the case of HIP)
 - debugging and performance analysis tools

CUDA/HIP Programming Model

- GPU accelerator is often called a *device* and CPU a *host*
- The programs are CPU centric
 - The CPU initializes the device, allocates GPU memory, and initiates the CPU-GPU transfers.
 - The CPU launches the kernel (parallel code) which is executed on a device by several threads.
- The kernels are written from the point of view of a single thread
 - Each thread has a unique ID

Hello World

```
#include <hip/hip_runtime.h>
#include <stdio.h>

int main(void){
    int count, device;

    hipGetDeviceCount(&count);
    hipGetDevice(&device);

    printf("Hello! I'm GPU %d out of %d GPUs in total.\n", device, count);
    return 0;
}
```

Vector Addition

```
__global__ void vector_add(float *A, float *B, float *C, int n){  
    int tid = threadIdx.x + blockIdx.x * blockDim.x;  
    if(tid<n){  
        C[tid] = A[tid]+B[tid];  
    }  
}
```

```
#include <hip/hip_runtime.h>  
#include <stdio.h>  
#include <stdlib.h>  
#include <math.h>  
int main(){  
    const int N = 10000;  
    float *Ah, *Bh, *Ch, *Cref;  
    float *Ad, *Bd, *Cd;  
  
    // Allocate the arrays on CPU  
    Ah =(float*)malloc(n * sizeof(float));Bh =...;Ch =...; Cref =...;  
  
    // Initialise data and calculate reference values on CPU  
    for (i=0; i < n; i++) {  
        Ah[i] = sin(i) * 2.3;  
        Bh[i] = cos(i) * 1.1;  
        Cref[i] = Ah[i] + Bh[i];}
```

```
// Allocate the arrays on GPU  
hipMalloc((void**)&Ad, N * sizeof(float));  
hipMalloc((void**)&Bd, N * sizeof(float));  
hipMalloc((void**)&Cd, N * sizeof(float));  
  
// Transfer the data from CPU to GPU  
hipMemcpy(Ad, Ah, sizeof(float) * n, hipMemcpyHostToDevice);  
hipMemcpy(Bd, Bh, sizeof(float) * n, hipMemcpyHostToDevice);  
  
// define grid dimensions + launch the device kernel  
dim3 blocks, threads;  
threads=dim3(256,1,1);  
blocks=dim3((N+256-1)/256,1,1);  
  
//Launch Kernel  
//hipLaunchKernelGGL(vector_add, blocks, threads, 0, 0, Ad, Bd, Cd, 1  
vector_add<<< blocks, threads,0,0>>>(Ad, Bd, Cd, N);  
  
// copy results back to CPU  
hipMemcpy(Ch, Cd, sizeof(float) * N, hipMemcpyDeviceToHost);  
  
// Free the GPU arrays  
hipFree(Ad); hipFree(Bd); hipFree(Cd);  
  
printf("Result: %f %f %f \n", Ch[3], Ch[n-2], Ch[n-1]);
```


Vector Addition with Unified Memory

```
__global__ void vector_add(float *A, float *B, float *C, int n){
    int tid = threadIdx.x + blockIdx.x * blockDim.x;
    if(tid < n){
        C[tid] = A[tid] + B[tid];
    }
}
```

```
int main(){
    const int N = 10000;
    float *Ah, *Bh, *Ch, *Cref;

    // Allocate the arrays using Unified Memory
    hipMallocManaged((void **)&Ah, N * sizeof(float));
    hipMallocManaged((void **)&Bh, N * sizeof(float));
    hipMallocManaged((void **)&Ch, N * sizeof(float));
    hipMallocManaged((void **)&Cref, N * sizeof(float));

    // Initialise data and calculate reference values on CPU
    for (i=0; i < n; i++) {
        Ah[i] = sin(i) * 2.3;
        Bh[i] = cos(i) * 1.1;
        Cref[i] = Ah[i] + Bh[i];
    }
    // All data at this point is on CPU
```

```
// define grid dimensions + launch the device kernel
dim3 blocks, threads;
threads = dim3(256, 1, 1);
blocks = dim3((N + 256 - 1) / 256, 1, 1);

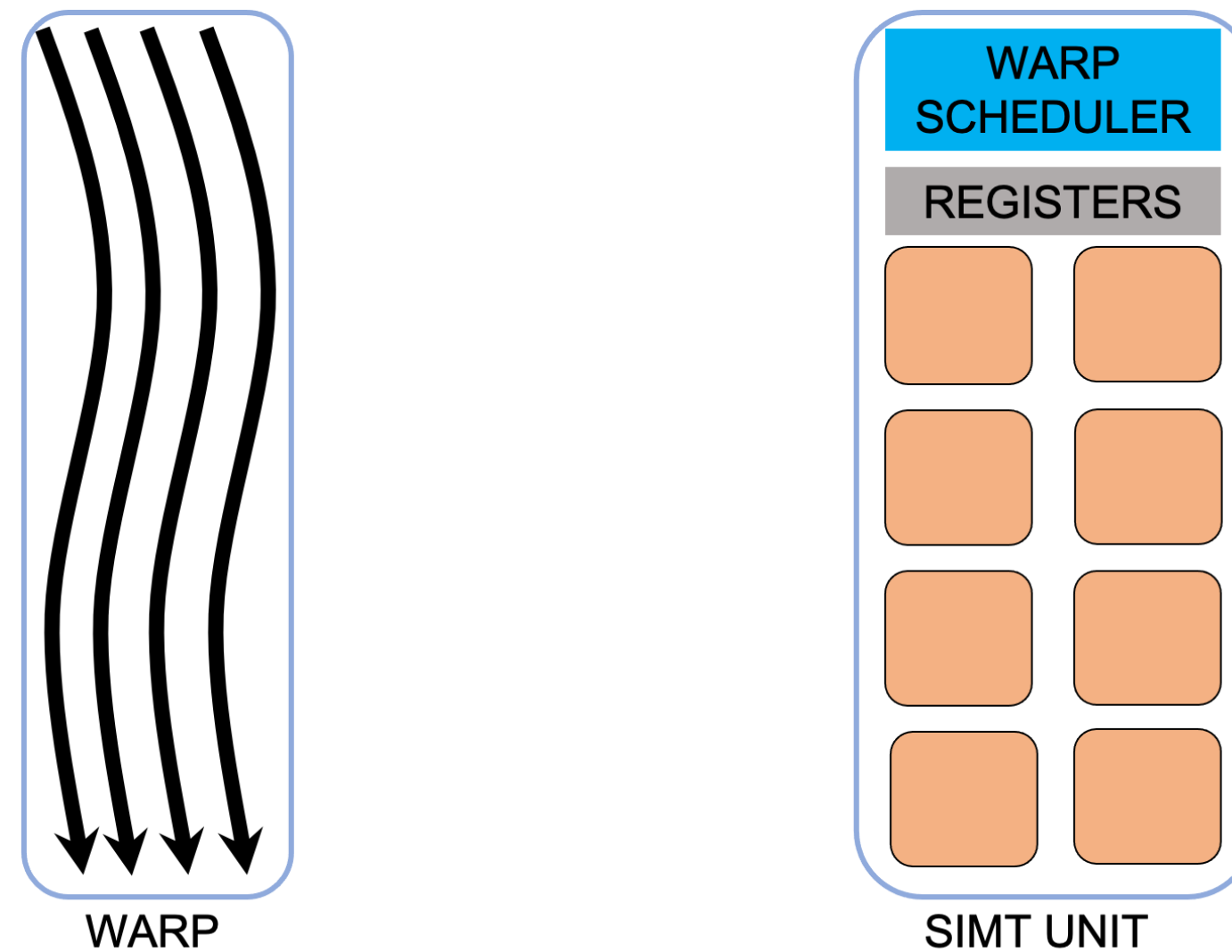
// Launch Kernel
// hipLaunchKernelGGL(vector_add, blocks, threads, 0, 0, Ah, Bh, Ch, N);
vector_add<<< blocks, threads, 0, 0>>>(Ah, Bh, Ch, N);
hipDeviceSynchronize(); // Wait for the kernel to complete

// Access the data on the CPU
printf("Result: %f %f %f \n", Ch[3], Ch[n-2], Ch[n-1]);

// Free the Unified Memory arrays
hipFree(Ah);
hipFree(Bh);
hipFree(Ch);
hipFree(Cref);
```

Non-portable kernel-based models. Memory optimizations

Coalesced Access



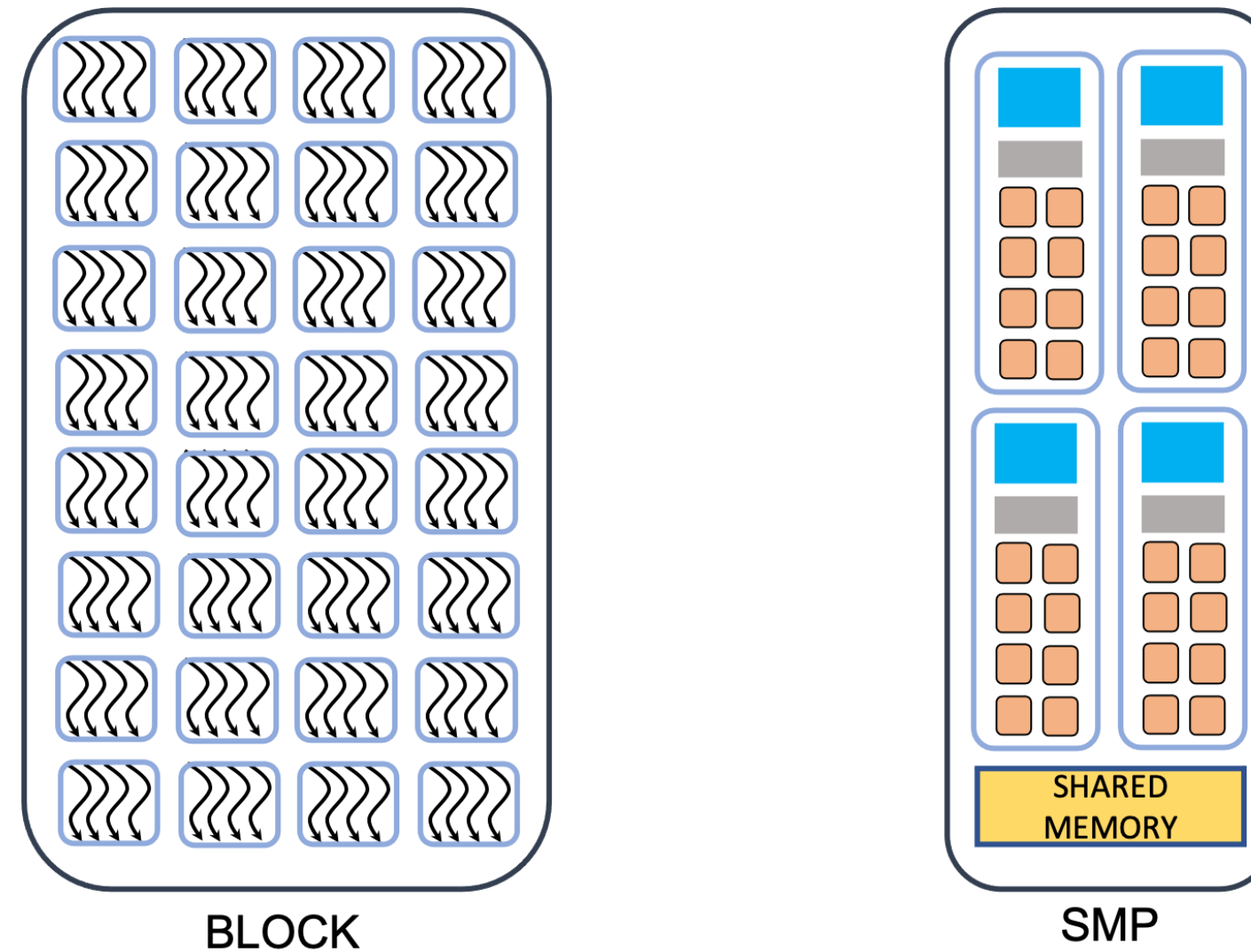
- The CUDA threads are physically locked into **warps**, currently of size 64 for AMD and 32 for Nvidia.
- All threads in the **warp** have to execute the same instruction.
- The memory accesses are done per warp.

Coalesced vs Non-coalesced Memory Access

```
__global__ void vector_add(float *A, float *B, float *C, int n, int stride, int shift){  
    int tid = threadIdx.x + blockIdx.x * blockDim.x;  
    if(tid < n){  
        C[tid] = A[tid] + B[tid]; //Coalesced  
  
        C[tid*stride] = A[tid*stride] + B[tid*stride]; //Strided Non-Coalesced  
  
        C[tid+shift] = A[tid+shift] + B[tid+shift]; //Shifted Non-Coalesced  
    }  
}
```

- Local shared memory can be used to improve the memory accesses.

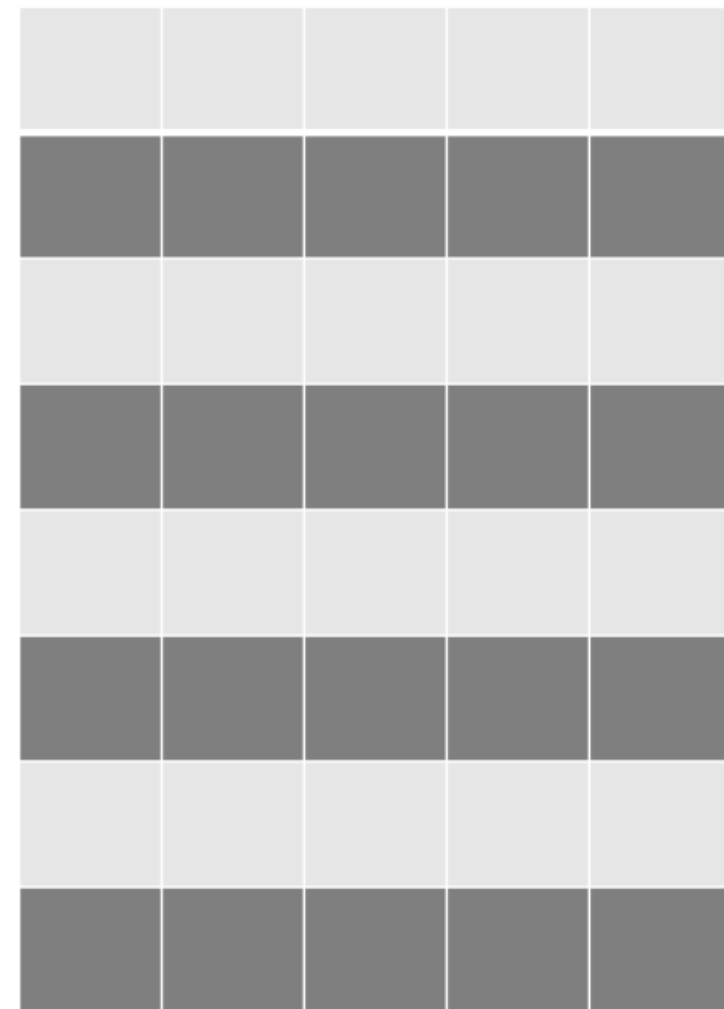
Block of Threads and Local Shared Memory



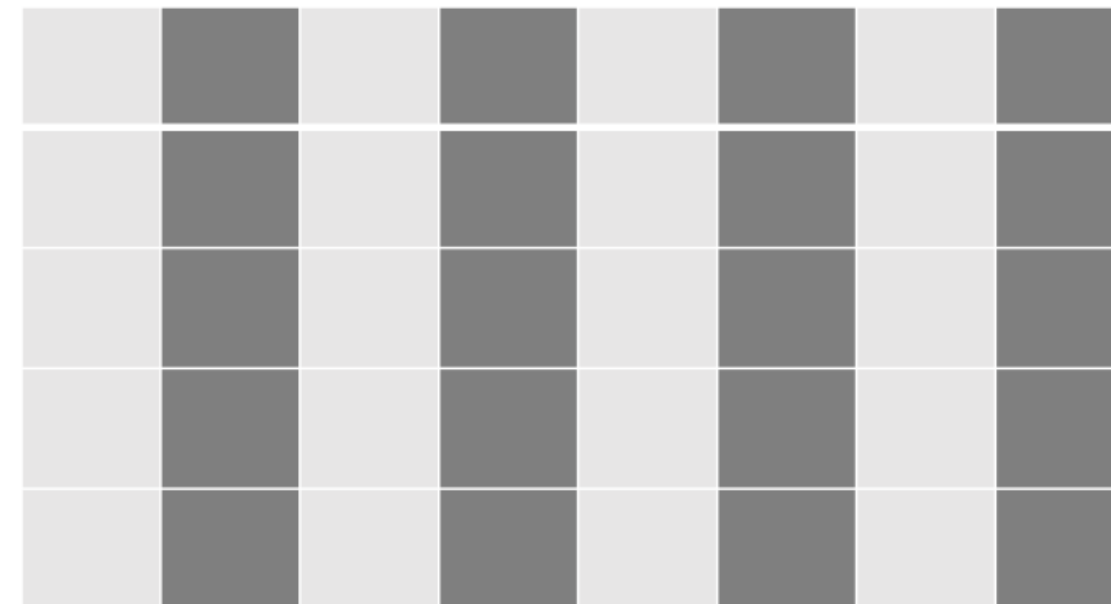
- Each block is assign to a SMP and it can not be split.
- Synchronization and data exchange is possible inside a block.

Optimizing matrix operations. $B(i, j) = A(j, i)$

NxM



MxN



Copy operation as base

```
__global__ void copy_kernel(float *in, float *out, int width, int height) {  
    int x_index = blockIdx.x * tile_dim + threadIdx.x;  
    int y_index = blockIdx.y * tile_dim + threadIdx.y;  
  
    int index = y_index * width + x_index;  
  
    out[index] = in[index];  
}
```

```
int block_x = width / tile_dim;  
int block_y = height / tile_dim;  
hipLaunchKernelGGL(copy_kernel, dim3(block_x, block_y),  
                    dim3(tile_dim, tile_dim), 0, 0, d_in, d_out, width,  
                    height);  
hipDeviceSynchronize();
```

The effective bandwidth is 717 GB/s, out of the theoretical peak 900 GB/s.

Matrix transpose naive

```
__global__ void transpose_kernel(float *in, float *out, int width, int height) {  
    int x_index = blockIdx.x * tile_dim + threadIdx.x;  
    int y_index = blockIdx.y * tile_dim + threadIdx.y;  
  
    int in_index = y_index * width + x_index;  
    int out_index = x_index * height + y_index;  
  
    out[out_index] = in[in_index];  
}
```

The effective bandwidth is 311 GB/s.

Matrix transpose with shared memory

```
__global__ void transpose_lds_kernel(float *in, float *out, int width,
                                     int height) {
    __shared__ float tile[tile_dim][tile_dim];

    int x_tile_index = blockIdx.x * tile_dim;
    int y_tile_index = blockIdx.y * tile_dim;

    int in_index =
        (y_tile_index + threadIdx.y) * width + (x_tile_index + threadIdx.x);
    int out_index =
        (x_tile_index + threadIdx.y) * height + (y_tile_index + threadIdx.x);

    tile[threadIdx.y][threadIdx.x] = in[in_index];

    __syncthreads();

    out[out_index] = tile[threadIdx.x][threadIdx.y];
}
```

The effective bandwidth is 674 GB/s.

Matrix transpose with shared memory without bank conflicts

```
__global__ void transpose_lds_kernel(float *in, float *out, int width,
                                   int height) {
    __shared__ float tile[tile_dim][tile_dim+1];

    int x_tile_index = blockIdx.x * tile_dim;
    int y_tile_index = blockIdx.y * tile_dim;

    int in_index =
        (y_tile_index + threadIdx.y) * width + (x_tile_index + threadIdx.x);
    int out_index =
        (x_tile_index + threadIdx.y) * height + (y_tile_index + threadIdx.x);

    tile[threadIdx.y][threadIdx.x] = in[in_index];

    __syncthreads();

    out[out_index] = tile[threadIdx.x][threadIdx.y];
}
```

On a NVIDIA V100 GPU this final code achieves an effective bandwidth 697 GB/s, out of the theoretical peak 900 GB/s.

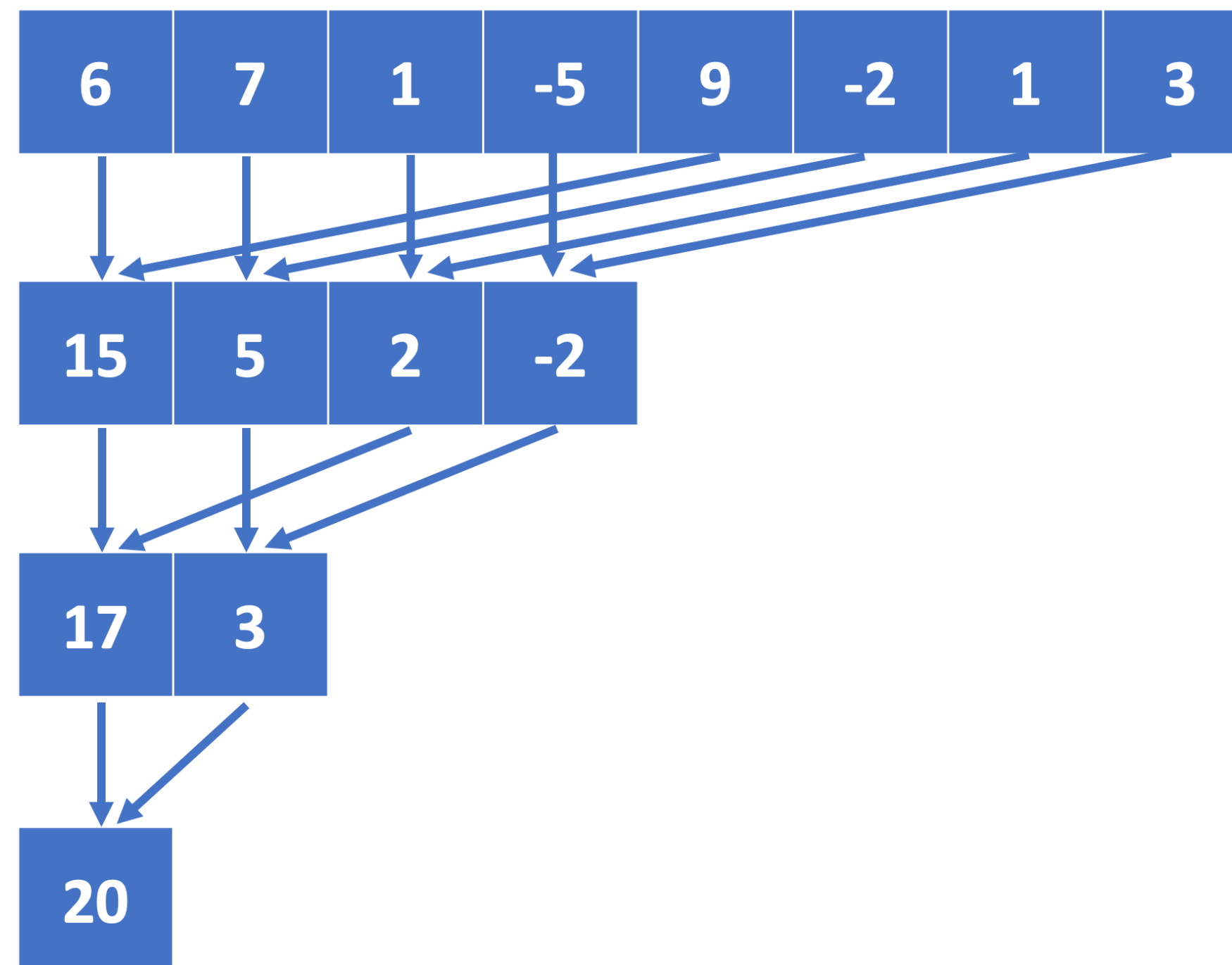
Reductions

- Reductions refer to operations in which the elements of an array are aggregated in a single value through binary operations.
- Examples include summing, finding the maximum or minimum, or performing logical operations.
- Assumptions for being able to perform them in parallel:
 - the order of the iterations does not change the results. $a+b=b+a$
 - doing the operations on small subsets, and then on the results does not change the results. $(a+b)+c=a+(b+c)$

Reduction in parallel

- Divide the problem in subsets which can be processed in parallel.
- Each subset is processed by a block of threads.
- Have an efficient reduction at block level:
 - keep as many as possible threads doing work.
 - avoid global memory accesses using local data share.

Tree Reduction Inside a Block of Threads



CUDA/HIP Reduction

```
#define tpb 512 // size in this case has to be known at compile time
// this kernel has to be launched with at least N/2 threads
__global__ void reduction_one(double x, double *sum, int N){
    int ibl=blockIdx.y+blockIdx.x*gridDim.y;
    int ind=threadIdx.x+blockDim.x*ibl;

    __shared__ double shtmp[2*tpb];
    shtmp[threadIdx.x]=0; // for sums we initiate with 0, for other operations should be different
    if(ind<N/2){
        shtmp[threadIdx.x]=x[ind];
    }
    if(ind+N/2<N){
        shtmp[threadIdx.x+tpb]=x[ind+N/2];
    }
    __syncthreads();
    for(int s=tpb;s>0;s>>=1){
        if(threadIdx.x<s){
            shtmp[threadIdx.x]+=shtmp[threadIdx.x+s];
        }
        __syncthreads();
    }
    if(threadIdx.x==0){
        sum[ibl]=shtmp[0]; // each block saves its partial result to an array
        // atomicAdd(&sum[0], shene[0]); // alternatively could aggregate everything together at index 0. Only use when there not many partial sums left
    }
}
```


CUDA/HIP Streams

- Modern GPUs can overlap independent operations.
- CPU-GPU data transfers can be overlapped with kernel execution.
- **CUDA/HIP streams** are independent execution units, a sequence of operations that execute in issue-order on the GPU.
- The operations issue in different streams can be executed concurrently.
- Utilizing multiple streams, the GPU can avoid idle time, especially for problems with frequent CPU communication or multi-GPU setups.

Overlapping Computations and Memory transfer

Time →

Serial Execution

H2D Engine		0			
Kernel Engine			0		
H2D Engine				0	

Concurrent Execution

H2D Engine		1	2	3	4	5			
Kernel Engine			1	2	3	4	5		
H2D Engine				1	2	3	4	5	

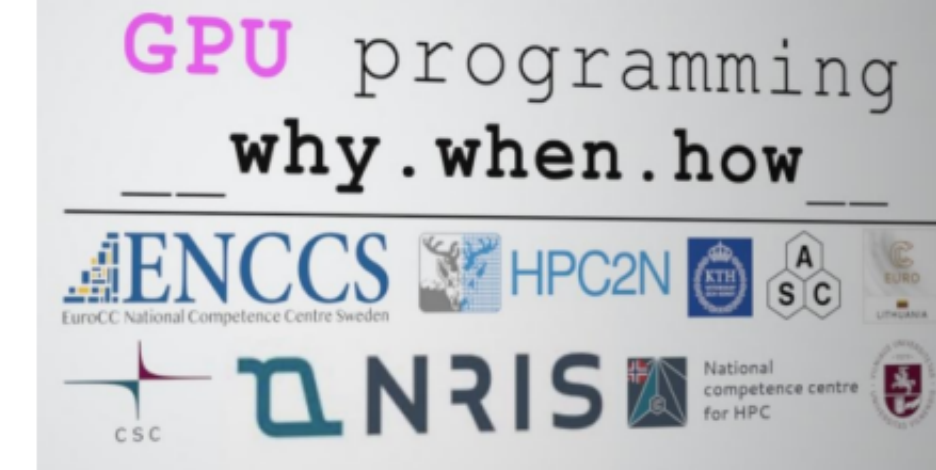
Vector Addition with Streams

```
// Distribute kernel for 'n_streams' streams, and record each stream's timing
for (int i = 0; i < n_streams; ++i) {
    int offset = i * (N/stream_size);
    hipEventRecord(start_event[i], stream[i]); // stamp the moment when the kernel is submitted on stream i

    hipMemcpyAsync( &Ad[offset], &Ah[offset], N/n_streams*sizeof(float), hipMemcpyHostToDevice, stream[i]);
    hipMemcpyAsync( &Bd[offset], &Bh[offset], N/n_streams*sizeof(float), hipMemcpyHostToDevice, stream[i]);
    vector_add<<<gridsize / n_streams, blocksize, 0, stream[i]>>>(&Ad[offset], &Bd[offset], &Cd[offset], N/n_streams); //each call processes N/n_streams
    hipMemcpyAsync( &Ch[offset], &Cd[offset], N/n_streams*sizeof(float), hipMemcpyDeviceToHost, stream[i]);

    hipEventRecord(stop_event[i], stream[i]); // stamp the moment when the kernel on stream i finished
}
...
```

Summary



- CUDA and HIP are the native programming models for NVIDIA and AMD GPUs.
- The programmer can take advantage of all GPU features.
- NVIDIA has a very extensive ecosystem. AMD is catching up.
- HIP is open source and can be used on both NVIDIA and AMD platforms.
- They are exclusive for NVIDIA and AMD GPUs.
- Both CUDA and HIP require learning GPU programming concepts.
- Memory optimizations are very important.